Strain-Induced Phase Transformations in Shape Memory Alloys

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Shape memory materials are characterized by the ability to generate large strains by applying moderate stresses with almost no plastic deformation. Above a structural transition temperature the deformation is completely recovered on removing the load. This behavior is also termed "pseudoelasticity." Some materials, such as NiTi alloys can recover strains up to 10%, making these materials suitable for a large number of technological applications. This property arises due to a strain-induced, diffusionless, shear-driven structural transformation. The transformation makes the stress-strain curves highly nonlinear and a plateau, analogous to plasticity, is observed. However, upon removing the load, the material transforms back to the parent crystal structure and all the deformation is recovered.

We have developed a framework to model the pseudoelasticity of these materials, in particular FePd which undergoes a cubic to tetragonal transformation. The modeling is based on continuum elasticity with a nonlinear elastic free energy. The free energy is written as an expansion in the components of the strain tensor. The main criterion in constructing this free energy expansion is that the underlying point group symmetry of the crystal is satisfied. The dynamics and microstructural evolution are simulated by using force balance equations for the displacement fields. Dissipation is accounted for by a viscous damping force in terms of the strain rates. The displacement field method ensures that elastic compatibility relations are automatically satisfied.

All parameters in the free energy are fitted to FePd experimental data for elastic constants, lattice parameters, phonon dispersion, and mobilities. The equations of motion are numerically solved on a 64 x 32 x 32 grid using finite differences and periodic boundary conditions are assumed. Preliminary results for small systems that simulate a block of material .08*.04*.04 μm^3 for roughly several nanoseconds, with a uniaxial strain loading at a rate of $10^6/s$, are shown in Fig. 1. The microstructure in terms of strains is shown at a point on the stress-strain curve. Note how the system nucleates domain walls on overcoming a barrier to the formation of tetragonal variants. This barrier decreases as the strain rate decreases. These simulations allow us to understand the influence of strain rate on nucleation processes at the mesoscale. Our work is currently being applied to materials that transform from cubic to orthorhombic (CuAlNi, U6Nb) and cubic to monoclinic (NiTi, Pu), as some of these materials are of strategic interest to Nuclear Weapons programs.

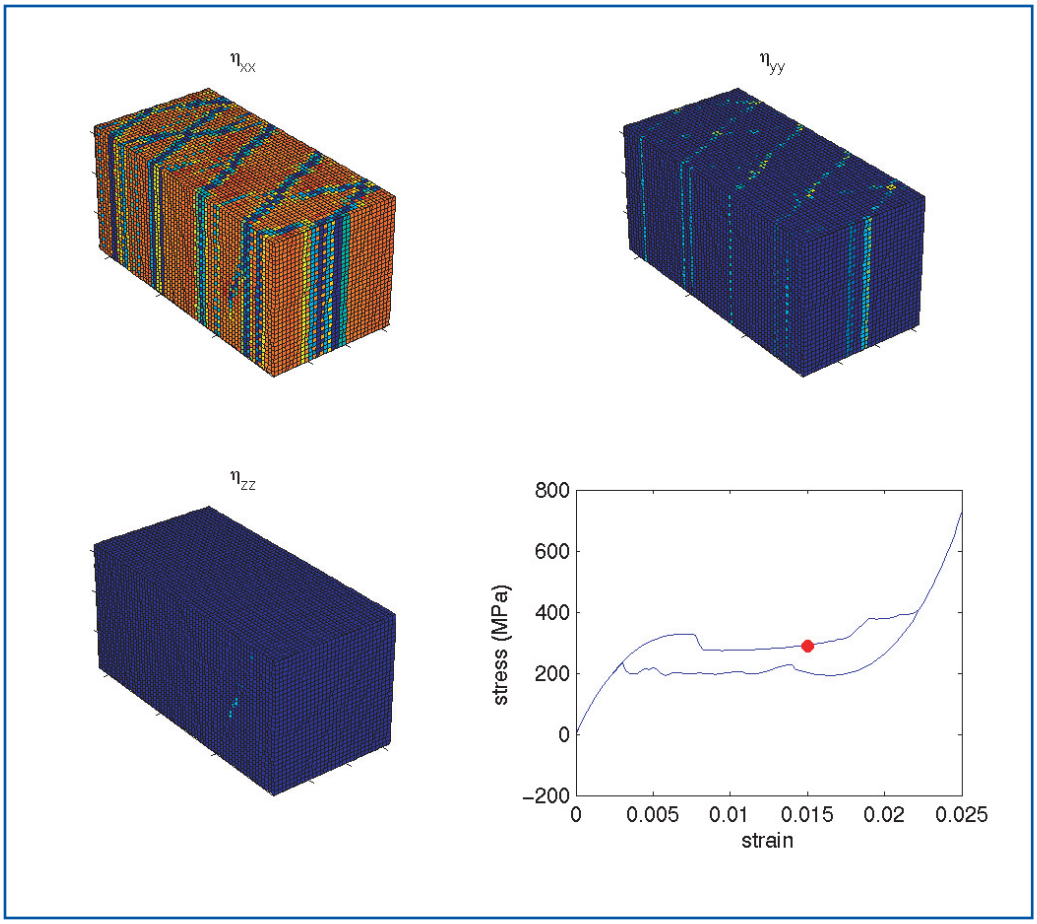

Figure 1—
Strain tensor components η_{xx}, η_{yy}, η_{zz} at a given point on the stress-strain curve. Red corresponds to large positive values and blue to zero. The strain loading is in the direction of the tetragonal variant along the x direction.